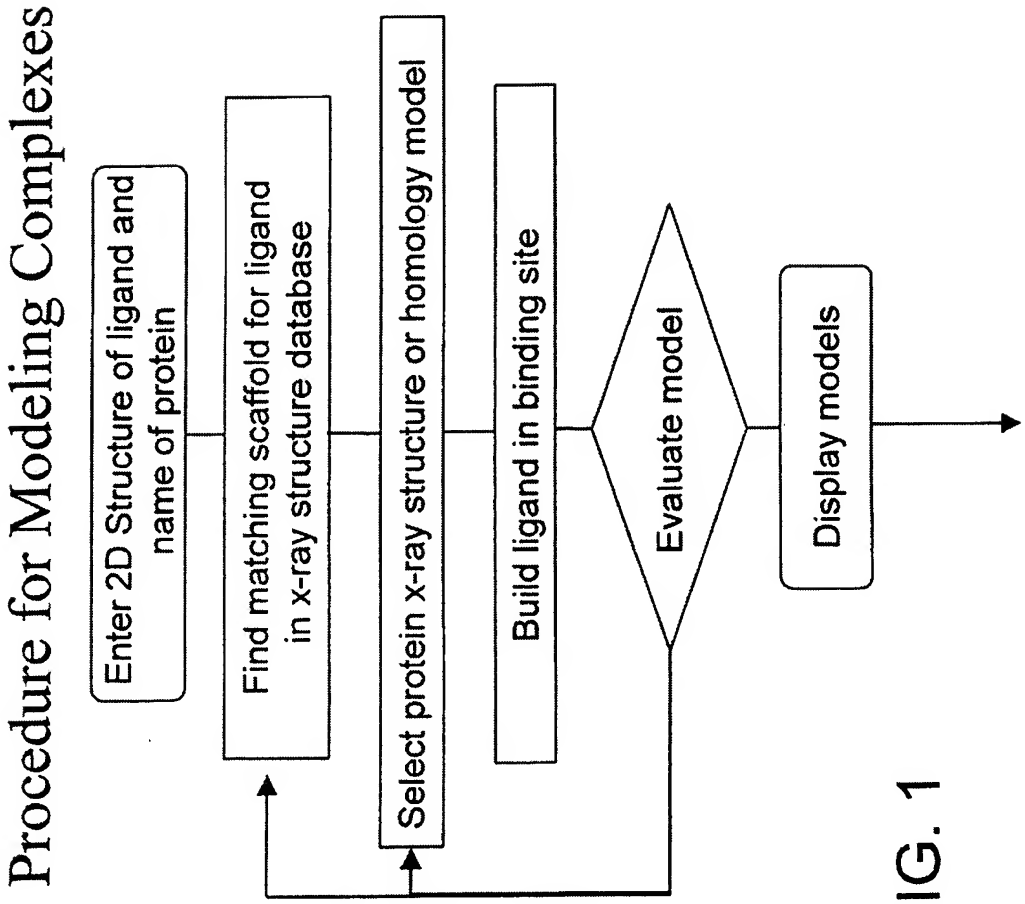

Procedure for Modeling Complexes
Enter 2D Structure of ligand and name of protein
Find matching scaffold for ligand in x-ray structure database
Select protein x-ray structure or homology model
Build ligand in binding site
Evaluate model
Display models

FIG. 1

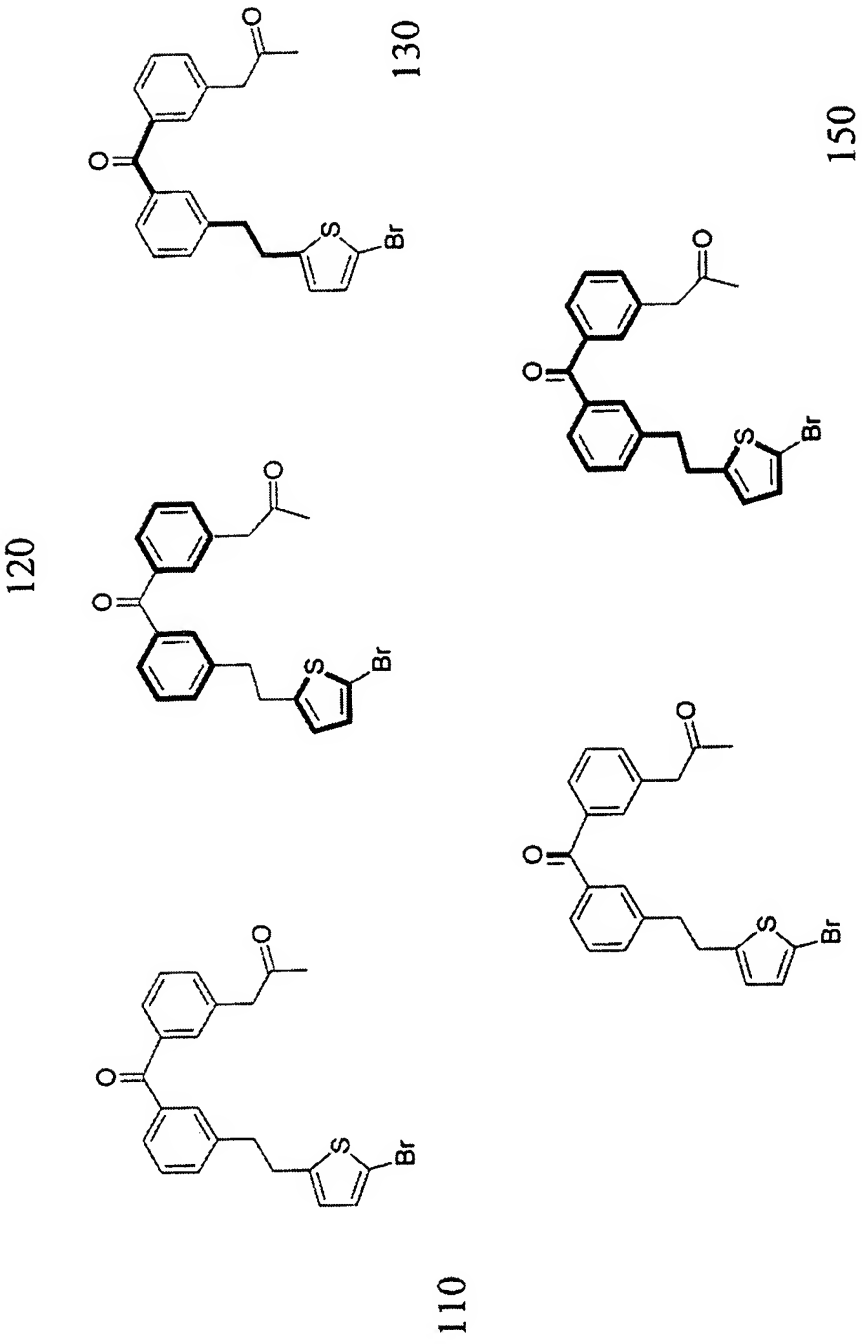


FIG. 2

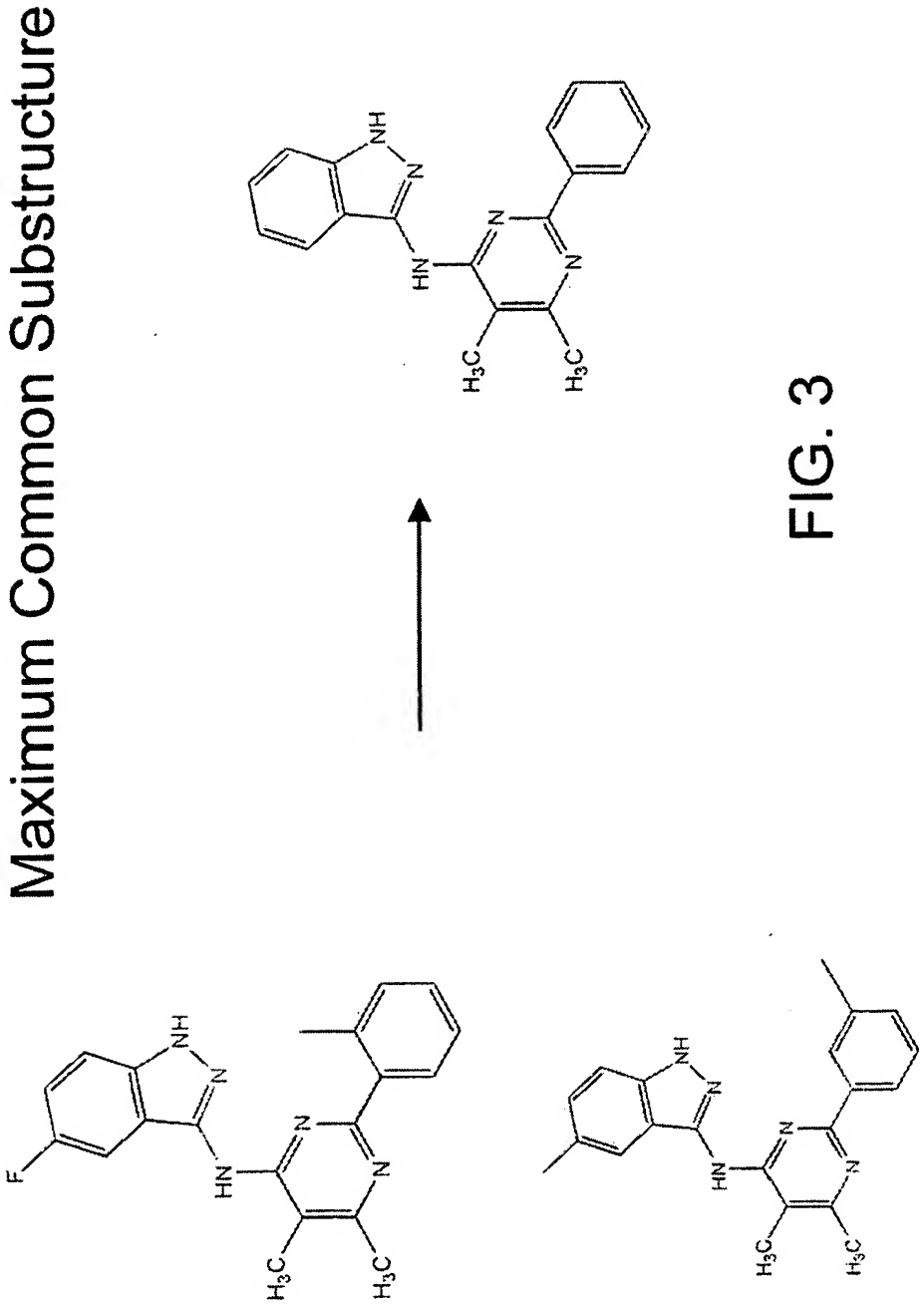


FIG. 3

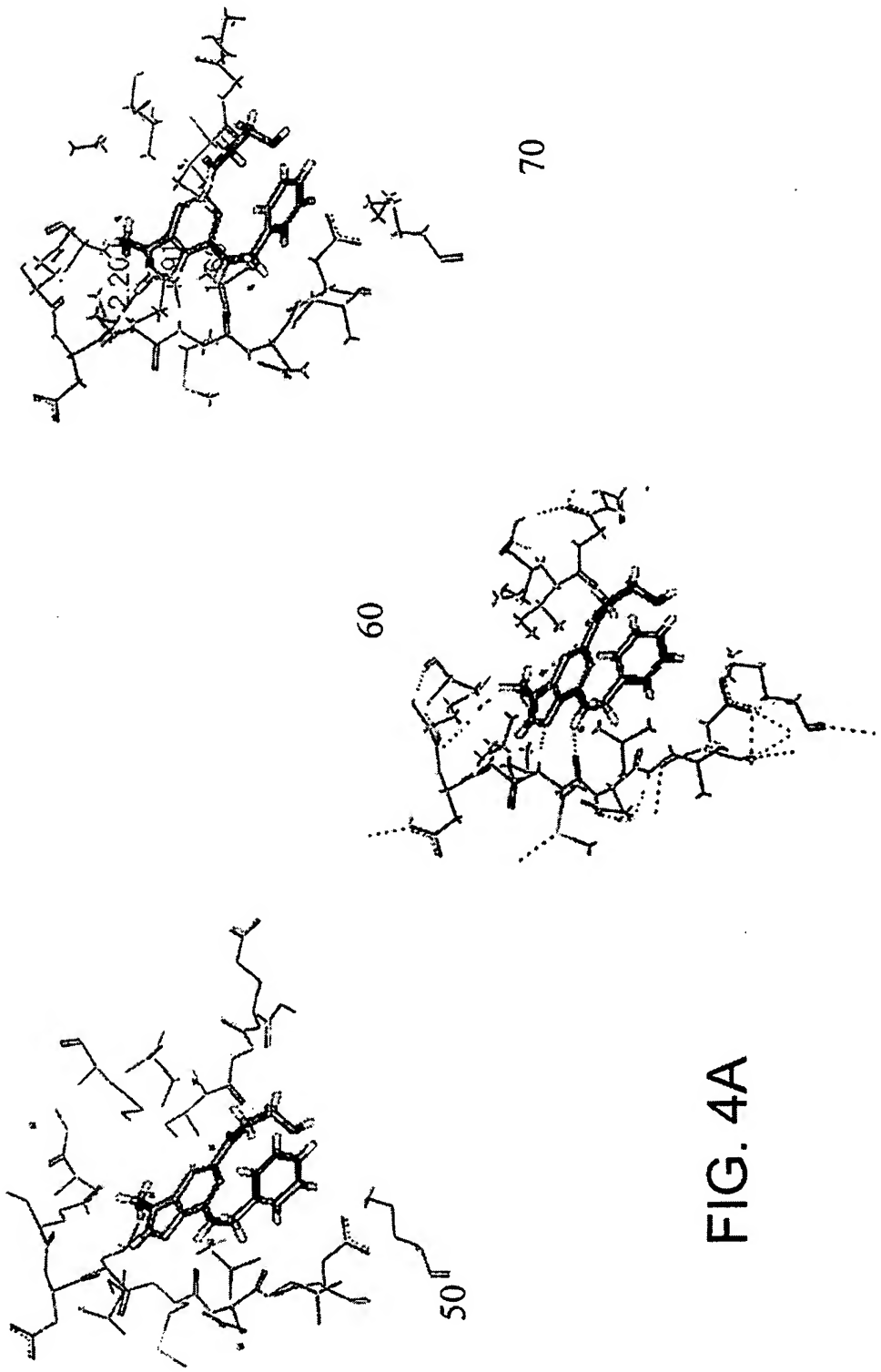
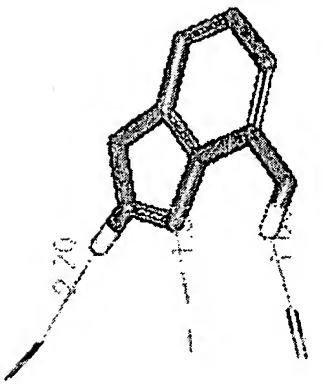
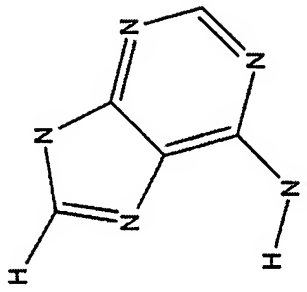


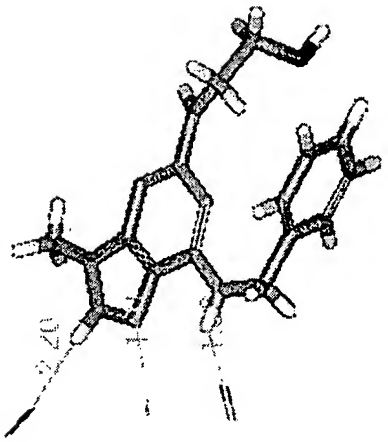
FIG. 4A



90



100



80

FIG. 4B

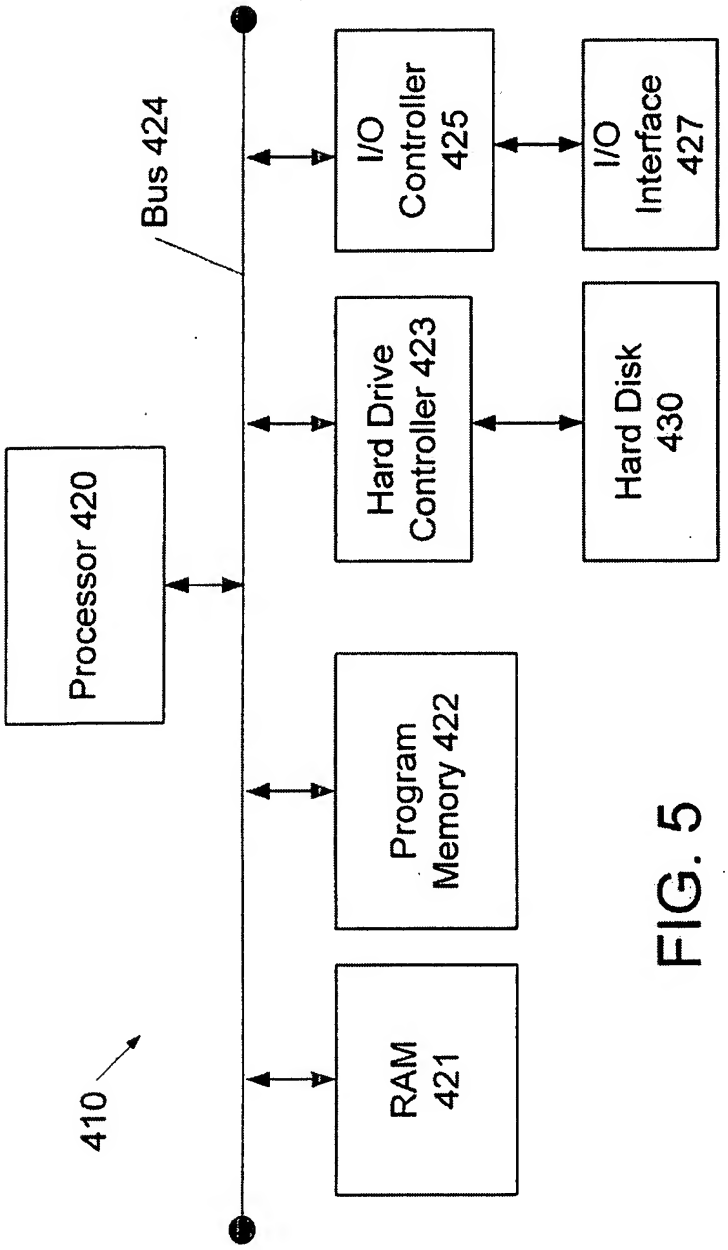

Bus 424
I/O Controller 425
I/O Interface 427
Hard Drive Controller 423
Hard Disk 430
Processor 420
Program Memory 422
RAM 421
410

FIG. 5

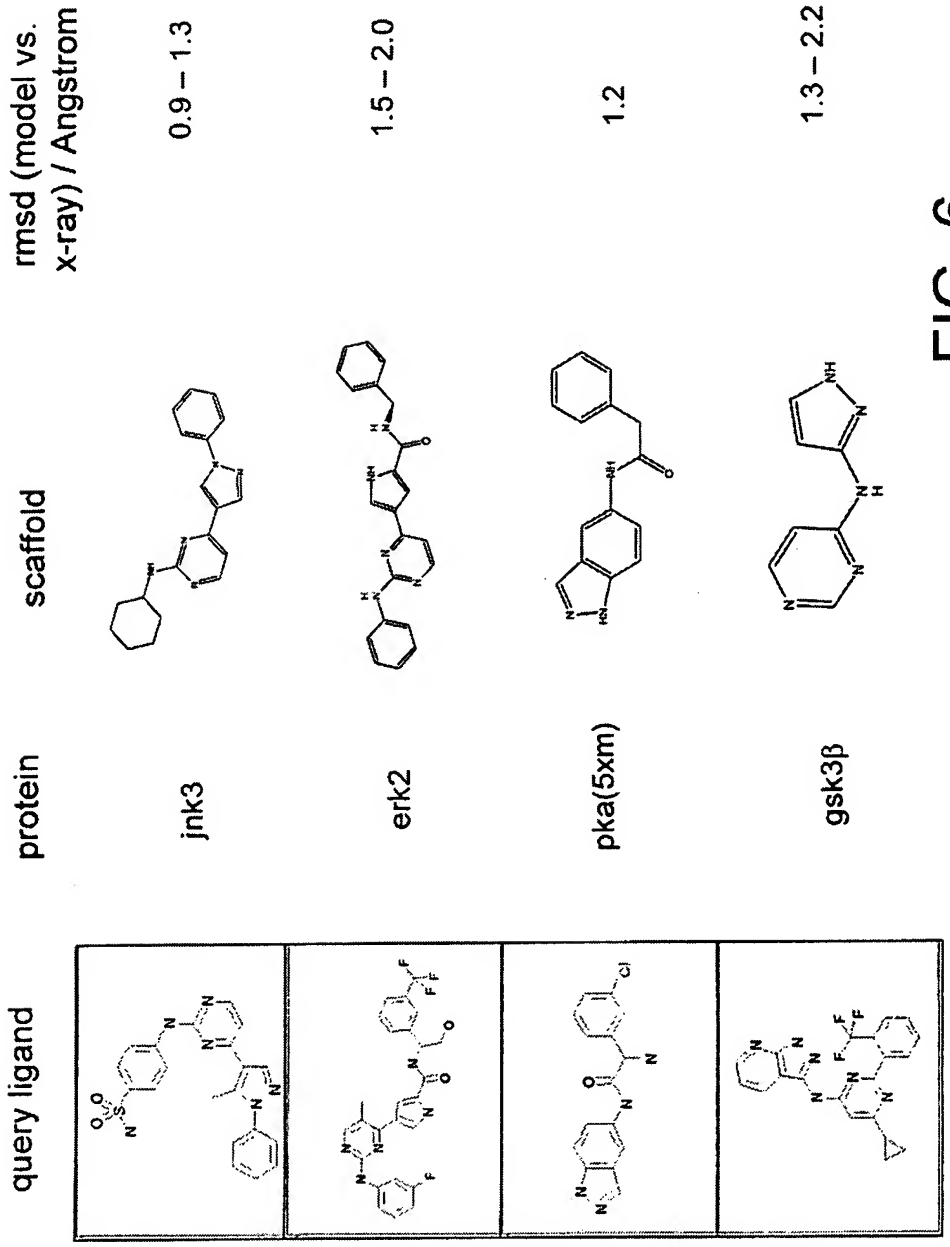

query ligand
protein
scaffold
rmsd (model vs. x-ray) / Angstrom
jnk3
0.9 – 1.3
erk2
1.5 – 2.0
pka(5xm)
1.2
gsk3β
1.3 – 2.2

FIG. 6

T1 – 17 ATOMS

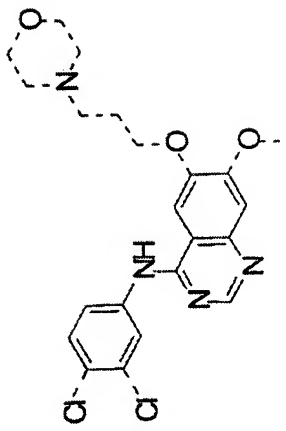


FIG. 7A

T2 – 11 ATOMS

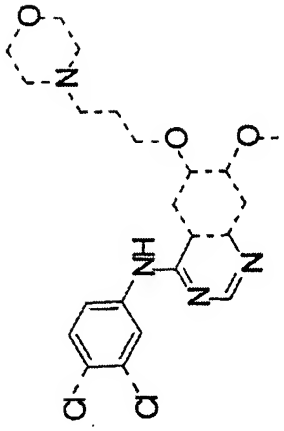


FIG. 7B

T3 –10 ATOMS

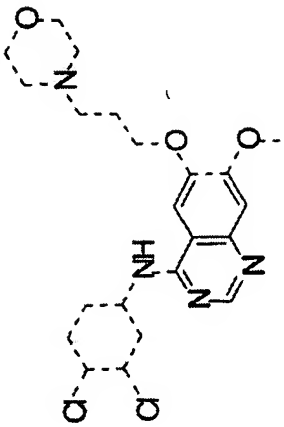


FIG. 7C

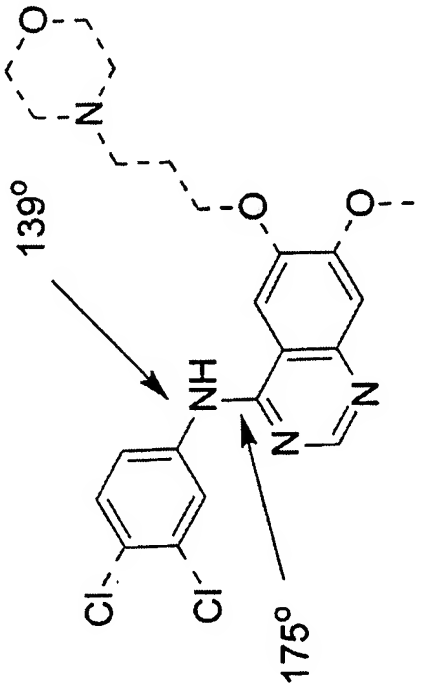


FIG. 8

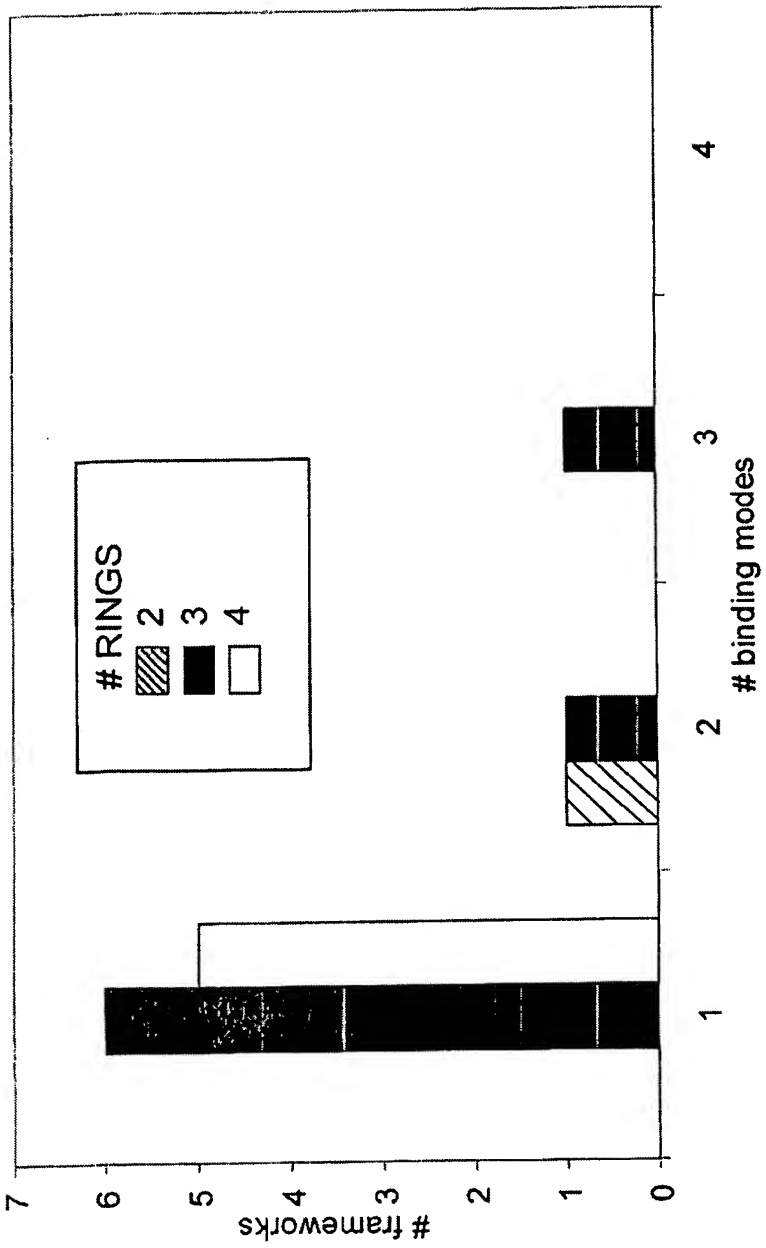


FIG. 9

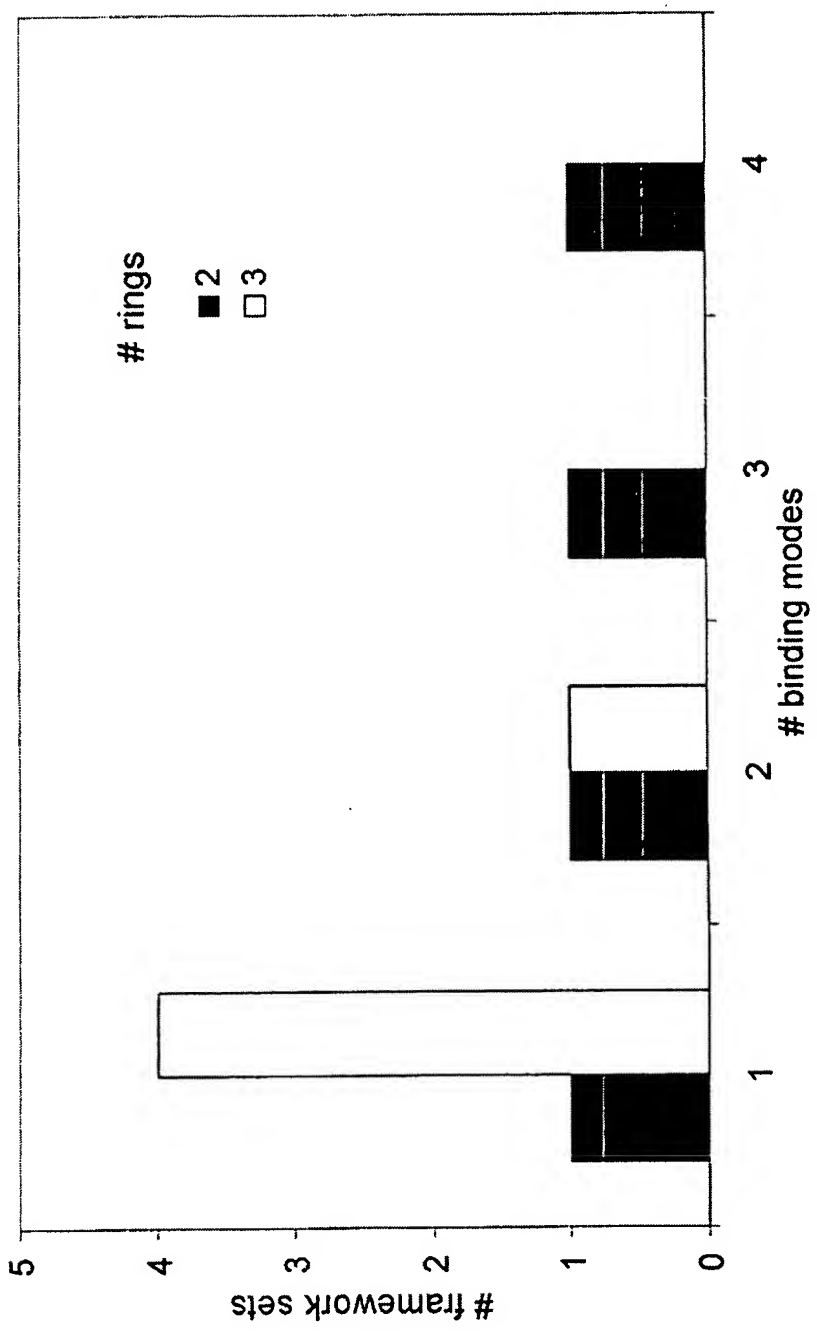


FIG. 10

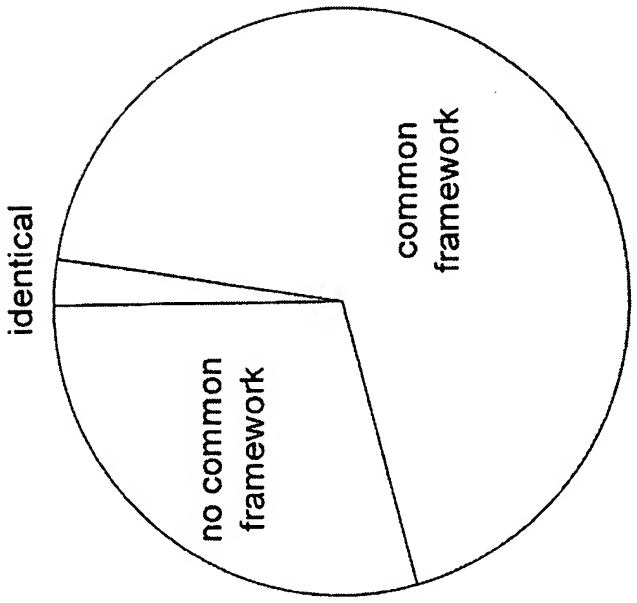


FIG. 11

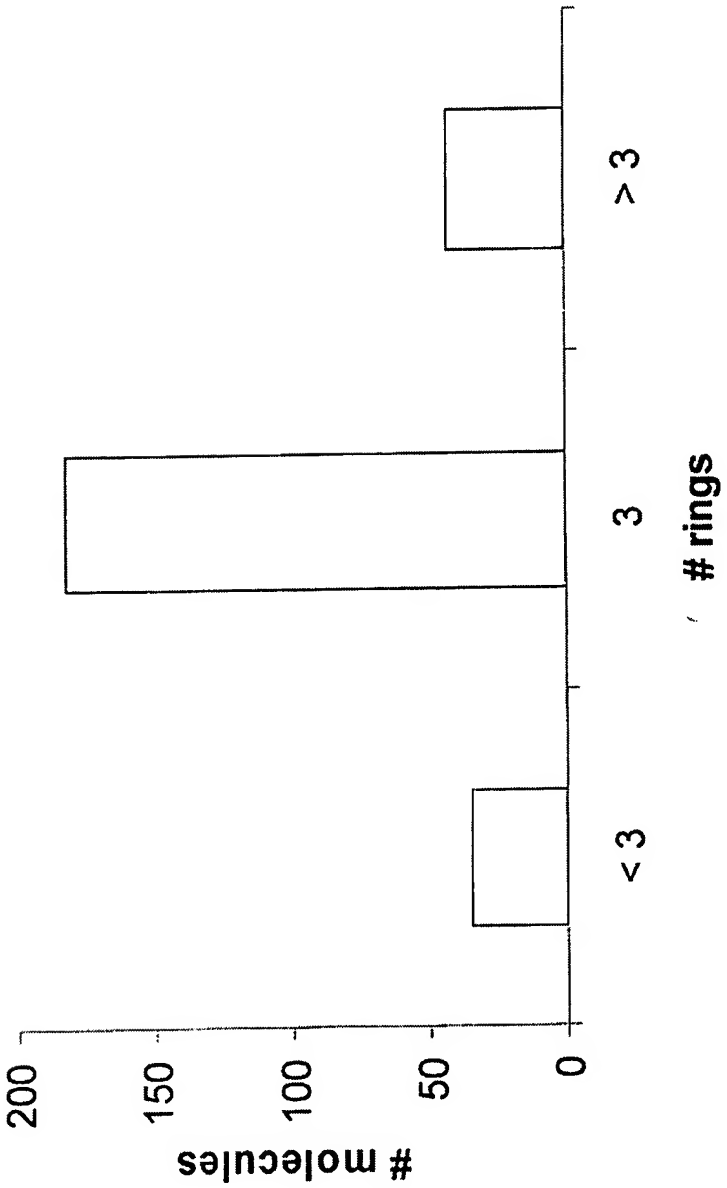
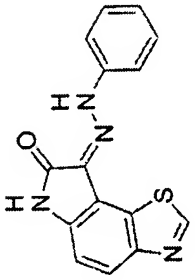
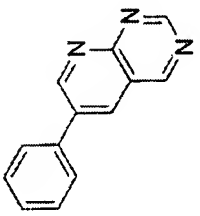


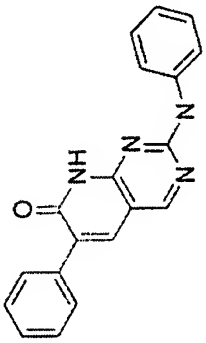
FIG. 12



10



9



8

FIG. 13